

**NSLINK**  
**NJOY-SCALE-LINK**

**User's Manual**

P.F.A. de Leege

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# PROGRAM ABSTRACT

1. NAME OR DESIGNATION OF PROGRAM - NSLINK
2. COMPUTER FOR WHICH THE PROGRAM IS DESIGNED AND OTHER MACHINE PACKAGES AVAILABLE -

Program_name	Package-ID	Orig. Computer	Test Computer
NSLINK		DEC VAX 8350	DEC VAXCLUSTER

3. DESCRIPTION OF PROGRAM OR FUNCTION - NSLINK (NJOY - SCALE - LINK) is a set of computer codes to couple the NJOY cross-section generation code to the SCALE-3 code system (using AMPX-2 master library format) retaining the Nordheim resolved resonance treatment option.

4. METHOD OF SOLUTION - The following module and codes are included in NSLINK:

**XLACSR:** This module is a stripped-down version of the XLACS-2 code. The module passes all  $\ell=0$  resonance parameters as well as the contribution from all other resonances to the group cross-sections, the contribution from the wings of the  $\ell=0$  resonances, the background cross-section and possible interference for multilevel Breit-Wigner resonance parameters. The group cross-sections are stored in the appropriate 1-D cross-section arrays. The output file has AMPX-2 master format. The original NJOY code is used to calculate all other data. The XLACSR module is included in the NJOY code.

**MILER:** This code converts NJOY output (GENDF format) to AMPX-2 master format. The code is an extensively revised version of the original MILER code. In addition, the treatment of thermal scattering matrices at different temperatures is included.

**UNITABR:** This code is a revised version of the UNITAB code. It merges the output of XLACSR and MILER in such a way that contributions from the bodies of the  $\ell=0$  resonances in the resolved energy range, calculated by XLACSR, are subtracted from the 1-D group cross-section arrays for fission (MT=18) and neutron capture (MT=102). The  $\ell=0$  resonance parameters and the contributions from the bodies of these resonances are added separately (MT=1023, 1022 and 1021). The total cross-section (MT=1), the absorption cross-section (MT=27) and the neutron disappearance cross-section (MT=101) values are adjusted.

In the case of Bondarenko data, the infinite dilution values of the cross-sections (MT=1, 18 and 102) are changed in the same way as the 1-D cross-sections.

The output file of UNITABR is in AMPX-2 master format and includes Nordheim parameters or Bondarenko and Nordheim parameters for the resonance treatment in BONAMI and/or NITAWL, which are codes of the SCALE system.

**BONAMI:** In order to take into account the combination of Bondarenko and Nordheim resonance treatment, certain subroutines are included in the package which replace some subroutines in the BONAMI code.

**5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM.**

6. **TYPICAL RUNNING TIME** – A sample problem ( $^{235}_{92}\text{U}$ ) with 187 neutron groups and Legendre polynomial order 3 (P3), requires on a DEC VAXstation 3100 (model 30) for XLACSR ~8 minutes; MILER ~80 seconds and UNITABR ~8 seconds.
7. **UNUSUAL FEATURES OF THE PROGRAM** – The present version of the code package is designed for the NJOY87 code. It can be used with the NJOY89 code as well, by a minor change of the main routine of NJOY89 (add 5 statements).
8. **RELATED AND AUXILIARY PROGRAMS** – AMPX-II modules (RADE, DIAL, CHOX, AIM, etc.) can be used to check, edit, couple, convert etc. the output files. Standard AMPX-II and NJOY subroutines and functions are widely used in NSLINK.

**9. STATUS –**

**10. REFERENCES –**

- R.E. MacFarlane and D.W. Muir  
NJOY87 – A Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B Evaluated Nuclear Data, PSR-171 (November 1987).
- N.M. Greene *et al.*  
AMPX – A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Libraries from ENDF/B, (March 1976).  
Revised to level of AMPX-II, ORNL/TM-3706 (December 1978).
- SCALE-3.1 - A modular Code System for Performing Standardized Computer Analyses for Licensing and Evaluation, CCC-466 (March 1985; July 1986).
- SCALIAS-3.1 - Selected FORTRAN 77 Modules from SCALE-3.1 (October 1986).
- N.M. Greene, private communication (November 1988).
- G.C. Panini  
MILER – Master Interface Library maker, abstract NEA 1198 (July 1988).

11. **MACHINE REQUIREMENTS** – XLACSR requires ~1600 kbytes, MILER ~800 kbytes and UNITABR ~400 kbytes of core memory on a VAX computer. Depending on the input choice the following scratch disc space is necessary: XLACSR ~200 kbytes; MILER ~40 Mbytes and UNITABR ~600 kbytes.

**12. PROGRAMMING LANGUAGE USED.**

FORTRAN 77

**13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED –**  
VAX/VMS 5.3

**14. ANY OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS.**

**15. NAME AND ESTABLISHMENT OF AUTHOR -**

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**16. MATERIAL AVAILABLE -**

NJOY87 main source (FORTRAN)  
XLACSR source (FORTRAN)  
MILER (extensively revised) source (FORTRAN)  
UNITABR source (FORTRAN)  
BONAMI subroutines (BFEDIT, CAPY, MAST and SELECT) source (FORTRAN)  
Sample problem 1 input file NJOY87  
Sample problem 2 input file NJOY87 including XLACSR  
Sample problem 1 and 2 input file MILER  
Sample problem 2 input file UNITABR  
Sample problem 1 output file NJOY87  
Sample problem 2 output file NJOY87 including XLACSR  
Sample problem 1 output file MILER  
Sample problem 2 output file MILER  
Sample problem 2 output file UNITABR  
Sample problem 1 and 2 command file NJOY87 (including XLACSR)  
Sample problem 1 and 2 command file MILER  
Sample problem 2 command file UNITABR

**17. CATEGORY. B M**

**KEYWORDS -**

cross sections, Nordheim resonance treatment, data processing, libraries, multigroup

# Contents

1	Introduction .....	4
2	General remarks .....	6
3	XLACSR.....	7
4	MILER .....	8
5	UNITABR .....	11
6	BONAMI .....	13
7	Sample Problems.....	14
	References.....	15
	Appendix A.....	16
	Input data XLACSR.....	16
	Appendix B.....	17
	Command file (VAX/VMS) to run NJOY (including XLACSR) .....	17
	Appendix C .....	18
	NJOY input file for sample problem 1: hydrogen in water (different temperatures).....	18
	Appendix D .....	20
	NJOY input file for sample problem 2: $^{235}\text{U}$ , different temperatures and $\sigma_0$ values.....	20
	Appendix E.....	23
	Command file (VAX/VMS) to run MILER .....	23
	Appendix F .....	23
	MILER input file for sample problems 1 and 2 .....	23
	Appendix G .....	24
	Command file (VAX/VMS) to run UNITABR .....	24
	Appendix H .....	24
	UNITABR input file for sample problem 2 .....	24
	Appendix I .....	25

Contents of tape .....	25
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## **Figures**

Figure 1. Flow diagram of NSLINK .....	5
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# 1 Introduction

The AMPX master library is organized into one- and two-dimensional arrays by reaction type, scattering expansion order and energy groups. Also, Bondarenko selfshielding parameters and Nordheim resonance parameters can be included in the library. The master library can be generated with the XLACS and XLACS-2 codes. However, the fine-group cross-sections generation code NJOY can treat different ENDF formats such as 4, 5 and 6. The code includes more advanced options, is well-maintained and internationally accepted.

In order to generate fine-group cross-sections with the NJOY<sup>1</sup> code and to put them in AMPX master library format, a set of computer codes named NSLINK (NJOY-SCALE-LINK) has been developed. In the AMPX master library, data is included for further processing according to the Nordheim resonance treatment. Bondarenko selfshielding parameters can be generated as well. Resonance calculations can be done with the Bondarenko, Nordheim or Bondarenko and Nordheim resonance treatment using the BONAMI and/or NITAWL codes from the SCALE-3<sup>2,3</sup> code package.

The following module and codes are included in the NSLINK package:

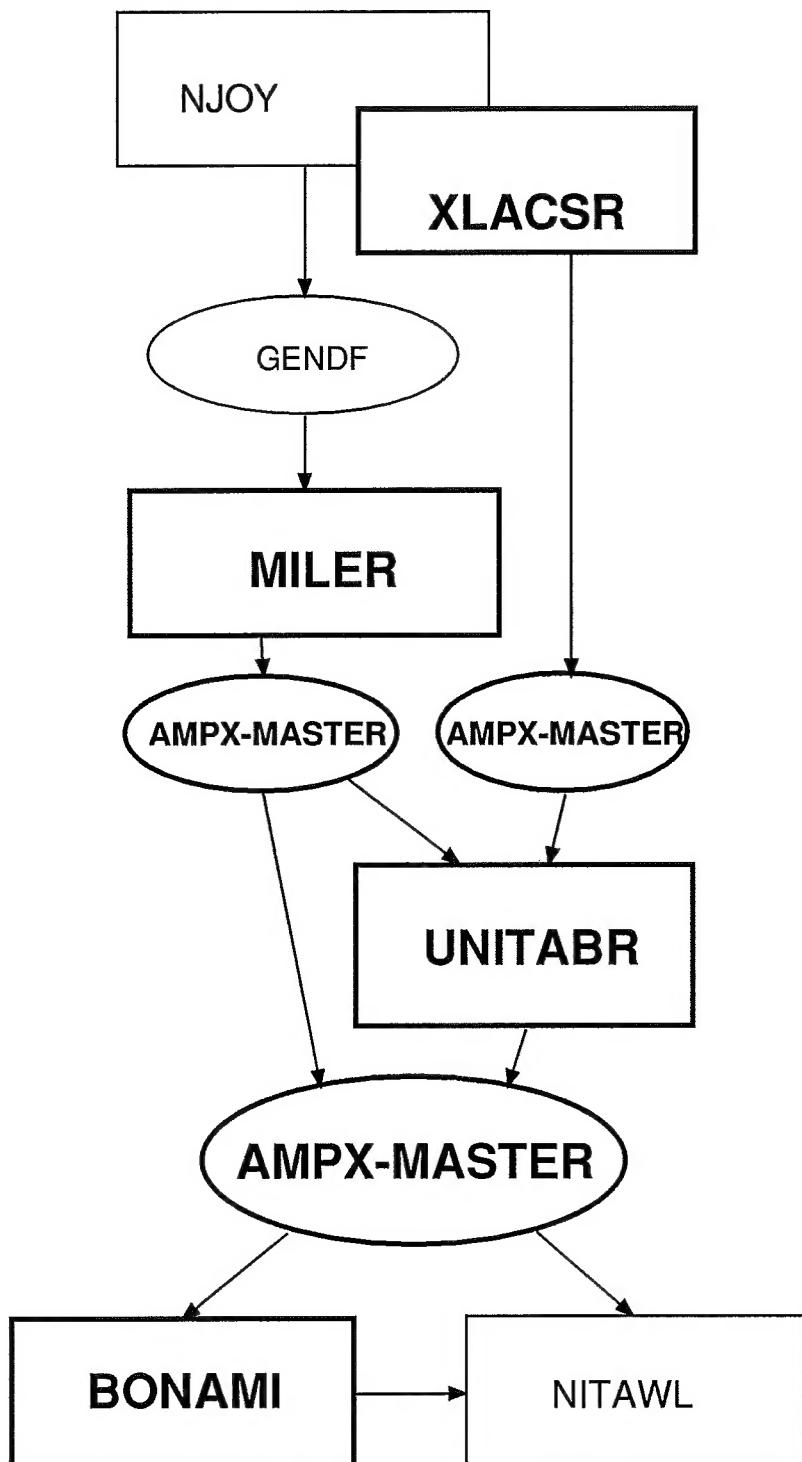
- XLACSR: This module (part of the NJOY code) is a stripped-down version of the XLACS-2<sup>4</sup> code. The necessary data for the Nordheim resonance treatment is generated by XLACSR.
- MILER: This code is an extensively revised version of the original MILER<sup>5</sup> code. MILER converts output from NJOY (ENDF format) to AMPX-2 master format.
- UNITABR: This code is an adapted version of the UNITAB<sup>4</sup> code. It merges the output of XLACSR and MILER.
- BONAMI: In order to combine Bondarenko and Nordheim resonance treatment, some revised subroutines of the BONAMI code are included which replace the original ones.

NSLINK is part of the INAS (IRI-NJOY-AMPX-SCALE) computer code package. The flow diagram of NSLINK is shown in figure 1.

The Netherlands Energy Research Foundation (ECN), in Petten, The Netherlands, contributed to the revision of MILER and tested the module and codes as well. They make use of NSLINK in the PASC (PETTEN-AMPX-SCALE) computer code package.

**Figure 1. Flow diagram of NSLINK**

Bold indicates: NSLINK



## 2 General remarks

The source code of NSLINK is written in FORTRAN 77; some system dependent code (input/output, precision of real values etc.) has been flagged ("CVAX", "CIBM" etc.).

Changes in the source code made by IRI are flagged "CIRI", changes made by ECN are flagged "CVE" or "CECN".

The ENDF-4, -5 and -6 formats can be used.

The NJOY87 or NJOY89 code can be used as well.

Only one nuclide can be processed per run.

The AMPX master library is generated in AMPX-2 master format and can only be used by AMPX-2 and SCALE-3 codes (NOT SCALE-4).

In some codes of AMPX and SCALE, the sequence of the treatment of Bondarenko selfshielding parameters and Nordheim resonance parameters is wrong if both are present. In the definition of the AMPX master format, the Bondarenko selfshielding parameters precede the Nordheim resonance parameters. In the AMPX utility codes AJAX, AIM, COMET, DIAL, MALOCS, RADE and UNITAB, the treatment of the Nordheim resonance parameters has to be done after the Bondarenko selfshielding parameters treatment. In most cases this can be easily accomplished by editing the FILE2 subroutine in these codes.

### 3 XLACSR

XLACSR is a stripped-down version of the XLACS-2<sup>4</sup> code. The module is included to generate the necessary data for the Nordheim resonance treatment in NITAWL. XLACSR passes all  $\ell=0$  resonance parameters as well as the contributions from all other resonances to the group cross-sections, the contribution from the wings of the  $\ell=0$  resonances, the background cross-sections and possible interference for multi-level Breit-Wigner resonance parameters. The group cross-sections are stored in the appropriate 1-D cross-section arrays. (MT=1, 2, 18, 102, and the bodies of the resonances 1021, 1022 and 1023) The output file has AMPX-2 master format.<sup>2,3,4</sup>

The original NJOY code is used to calculate all the data. The use of XLACSR does not affect the input to NJOY. In fact, if one does not want to use the Nordheim resonance treatment, the present NJOY version can still be used, with MILER to convert the output library of NJOY to the AMPX-2 master format. The XLACSR module is included in the NJOY code.

The module can be used by including the string \*XLACSR\* (version 87,89) or XLACSR (version 89) in the input stream of NJOY. The XLACSR input can be put anywhere in the NJOY input stream. The XLACS-2 input description (see Appendix A) can be used for XLACSR. Some input parameters have no meaning in the input stream for XLACSR (thermal treatment, scattering matrices etc.). The ENDF-4, -5 and -6 formats can be used.

XLACSR uses logical unit numbers in the range 90 thru 99 (other logical unit numbers are reserved for other modules in NJOY). The JEF or ENDF/B input library will be copied because of the read/write access in FORTRAN 77. After execution this copy will be deleted (see Appendix B: command file to run NJOY).

In Appendix D a sample input file for NJOY, including the XLACSR input, is shown. In the case of generating data for a nuclide with Bondarenko selfshielding parameters and Nordheim resonance parameters, the input stream for XLACSR must define the same group structure as for the GROUPR module in NJOY. Also, the same base (first) temperature must be selected. A value of  $10^{10}$  (infinite dilution) for  $\sigma_0$  is used.

## 4 MILER

The MILER<sup>5</sup> code converts a GENDF data library from NJOY to an AMPX-2 master format. Input instructions and definitions used to compute quantities in accordance with the definitions found in AMPX-2, are included as comment lines in the source code of MILER.

The code is revised extensively and some additions have been made<sup>a</sup>.

The most important revisions and additions are listed below:

- The use of MT=18 or MT=19 fission reaction type has been included.
- Revisions for the thermal scattering matrices.
  - If thermal scattering matrices are available (MT=201-230, or MT=221-236), all elastic scattering matrix elements (MT=2) in the thermal range are set to zero, because the elastic and thermal scattering matrices are added up in NITAWL.
  - The thermal scattering matrices contain some upscattering elements which express upscattering to the energy range above thermal. This will cause problems in MALOCS and NITAWL. The upscattering elements are deleted and the thermal scattering matrices are renormalized.
- It was found that after running NJOY, the resulting library sometimes contains zero cross-sections and all zero scattering matrix elements for some MT-numbers. This causes problems to the unmodified MILER. The modified MILER deletes all the MT-numbers with zero cross-sections and zero scattering matrix elements.
- The Bondarenko resonance treatment has been corrected.
- The initial setting of the directory for Bondarenko data in the AMPX-2 master is:
  - MT is the identifier of the process.
  - NF is the number of the first energy group for which parameters are given; set to one.
  - NL is the last group for which parameters are given; set to NMAX (the maximum number of groups).

<sup>a</sup>In co-operation with the Netherlands Energy Research Foundation (ECN), in Petten, The Netherlands

- ORDER is used to specify the order of the elastic scattering matrix (MT=2) if it is to be self-shielded; derived from input library.
- IOFF is the offset from the "magic-word" in the elastic scattering matrix; set to one.
- NZ is presently unused and has a value of zero.
- The use of the direct-access data file has been changed. In the records used, all the data is set to zero. (IBM mainframe computers initialize all the data in the records to zero)
- Thermal scattering matrices at different temperatures, as defined in the AMPX-2 master format, can be included in the AMPX master library. Two additional scratch units (15 and 16) are used in this case.

All these modifications are mainly in subroutines FILE3, FILE3T and FILE6. The subroutine FILE6T has been included.

The gamma production and/or photon interaction data conversion from GENDF format in AMPX-2 master format is not yet tested in this version of MILER!

Input specification, card 1:

- NIN0 is the GENDF input unit for all the temperature-independent neutron data, including the data for the first or base temperature as used in the Bondarenko resonance treatment. The thermal scattering matrices at the first (base) temperature are to be included as well (default=21).
- NINT is the GENDF input unit for all the temperature-dependent neutron data, including the data for the first or base temperature as used in the Bondarenko resonance treatment. The thermal scattering matrices at all temperatures are to be included as well (default=22).
- NOUT1 is the neutron (or photon) output unit (default=23).
- NOUT2 is the gamma production output unit (default=24).
- NDA is the scratch direct access unit (default=90).

Input specification, card 2:

- LOPT is the Legendre component of the neutron angular flux to be selected (0/1) (default=0).

See the examples in Appendix C and D (generation of temperature-dependent cross-sections with NJOY) and Appendix E and F (use of MILER).

## 5 UNITABR

This code is an adapted version of the original UNITAB<sup>4</sup> code which merges selected portions of AMPX master libraries into a new AMPX master library.<sup>6</sup>

- The output file of the XLACSR module (AMPX master format) is merged with the AMPX master file obtained from MILER (NJOY) in such a way that group cross-sections of the bodies of the  $\ell=0$  resonances in the resolved energy range (MT=1022 for fission and 1021 for capture), calculated by XLACSR, are subtracted from the infinite dilution values of the 1-D group cross-sections for fission (MT=18) and neutron capture (MT=102).
- The cross-sections of the bodies of the resonances (MT=1023 for elastic, 1022 and 1021) are added separately to the 1-D group cross-section arrays (MILER output).
- The redundant infinite dilution values of the total cross-sections (MT=1), the absorption cross-sections (MT=27) and the neutron disappearance cross-sections (MT=101) values are adjusted in the same way as for MT=18 etc..
- The  $\ell=0$  resonance parameters are included in the new AMPX master library.

In the case of Bondarenko selfshielding data:

- The total cross-section values in the 1-D group cross-section arrays are copied before adjustment and added to the 1-D arrays as well. The reaction type identification is MT=2000.
- The Bondarenko factors and infinite dilution values of the total cross-sections (MT=1) in the Bondarenko data part of the AMPX master library are copied (MT=2000) for special treatment in the BONAMI code.
- The infinite dilution values of the cross-sections (MT=1, 18 and 102) in the Bondarenko data part of the AMPX master library are adjusted in the same way as the cross-sections in the 1-D group cross-section arrays.

The input description of the original UNITAB code can be used with the following input data (underscored numbers are fixed):

- Coupling information (2 entries) 1\$\$:
  - NNNC (number of nuclides) is 1 (only one nuclide)
  - NCOM (number of coupling commands) is 2

- Coupling commands (2 lines of 4 entries) 2\$\$:
  - first line:
    - \* identifier of the nuclide in the new master data set
    - \* logical unit number of the device containing data from XLACSR ([\(23\)](#))
    - \* identifier of the nuclide in the master data set
    - \* "type" of data desired 5555 (Nordheim resonance parameters)
  - second line:
    - \* identifier of the nuclide in the new master data set (equal identifier in line 1)
    - \* logical unit number of the device containing data from MILER ([\(24\)](#))
    - \* identifier of the nuclide in the master data set
    - \* "type" of data desired 1111 (All neutron data)

The output file of UNITABR is in AMPX-2 master format and includes Nordheim resonance parameters or Bondarenko selfshielding parameters and Nordheim resonance parameters.

Do not use UNITABR to perform other options as described in the UNITAB manual !

See Appendix G and H for examples of the UNITABR command and input file.

## 6 BONAMI

BONAMI<sup>2,3</sup> is the code which performs the Bondarenko resonance treatment for the nuclides containing Bondarenko selfshielding parameters.

BONAMI allows the user to specify whether or not the code will iterate to determine the effective  $\sigma_0$  value from previously shielded total cross-sections for all groups and zones in the problem. In the non-iterative case, BONAMI uses the potential scattering cross-sections to determine the effective  $\sigma_0$  value.

The iteration starts with the infinite dilution values of the total cross-sections of the nuclides. With the NSLINK code system a nuclide may contain both Bondarenko self-shielding parameters and Nordheim resonance parameters. If Nordheim resonance parameters are available, the total cross-sections MT=1 cannot be used in the iterative process, because these cross-sections are adapted for the Nordheim resonance treatment to be performed later. Before correction, UNITABR copies the infinite dilution values of the total cross-sections and Bondarenko factors (MT=1 to MT=2000). If the total cross-sections MT=2000 are used instead of MT=1 this will be flagged in the printed output of BONAMI. If no Nordheim resonance parameters are available, the original iterative method is not affected.

Some revised subroutines are available which replace the original ones in BONAMI to take into account the treatment of the total cross-sections in the case of Nordheim resonance parameters. There are **no** changes in the BONAMI input description. The presence of the Nordheim resonance parameters in the AMPX master library will be detected by the BONAMI code.

The original input files for BONAMI can be used.

## 7 Sample Problems

Two sample problems are designed to demonstrate the options in the module and codes of NSLINK.

### 1. Example 1

In this example, cross-sections for hydrogen in water are generated. In particular, the generation of thermal scattering cross-sections and matrices is demonstrated at three different temperatures. The GROUPR module of NJOY has to be run twice; first to generate all temperature-independent data and, secondly, to generate all temperature-dependent data. The two output files from NJOY in GENDF format are input for the temperature-independent and temperature-dependent part of MILER. The command and input files (NJOY,MILER) are shown in Appendix B, C, E and F, respectively. MILER will generate a file in AMPX master format including thermal scattering matrices at three different temperatures

### 2. Example 2

In this example, cross-sections for  $^{235}\text{U}$  are generated. In particular, the generation of Bondarenko selfshielding parameters is demonstrated with three different values of  $\sigma_0$  and at three different temperatures. Thermal scattering cross-sections and matrices at three different temperatures are generated as well. The temperature used in the XLACSR input is equal to the first (base) temperature as used in the other input of NJOY. In both NJOY and XLACSR, the energy group structure has to be the same. As in example 1 the GROUPR module of NJOY has to be run twice; first to generate all temperature-independent data and, secondly, to generate all temperature-dependent data. The two output files from NJOY in GENDF format are input for the temperature-independent and temperature-dependent part of MILER. The output of MILER and XLACSR is input for the UNITABR code. The command and input files (NJOY(XLACSR), MILER and UNITABR) are shown in Appendix B, D, E, F, G and H, respectively. UNITABR will generate a file in AMPX master format including Nordheim resonance parameters or Bondarenko selfshielding parameters and Nordheim resonance parameters. Also, thermal scattering matrices at three different temperatures will be included.

The listings of the printed output files are available on magnetic tape as part of the code package documentation.

## References

1. R.E. MacFarlane and D.W. Muir  
NJOY87 - A Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B Evaluated Nuclear Data, PSR-171 (November 1987).
2. SCALE-3.1 - A modular Code System for Performing Standardized Computer Analyses for Licensing and Evaluation, CCC-466 (March 1985; July 1986).
3. SCALIAS-3.1 - Selected FORTRAN 77 Modules from SCALE-3.1, CCC-475 (October 1986).
4. N.M. Greene *et al.*  
AMPX - A Modular Code System for Generating Coupled Multigroup Neutron-Gamma libraries from ENDF/B, (March 1976). Revised to level of AMPX II, ORNL/TM-3706 (December 1978).
5. G.C. Panini  
MILER - Master Interface Library makER, abstract NEA 1198 (July 1988).
6. N.M. Greene, private communication (November 1988).

# **Appendix A**

## **Input data XLACSR**

The XLACS-2<sup>4</sup> input data can be used with the following comments:

- Data block 3 is not used.
- 2\$ array: IDTAP no meaning.
- 3\$ array: IOPT(2-6) no meaning.
- 70\$ array: LORDER, NL, NFY, MATID, KMXB and KMXA no meaning.
- 71\* array: MME, MMI and MATEL no meaning.
- 73\* Only one (base) temperature.
- The same energy boundaries as in NJOY must be used.
- No built-in group structures are available in XLACSR.
- The energy group boundaries are input (high-to-low) in eV.

## Appendix B

### Command file (VAX/VMS) to run NJOY (including XLACSR)

```
$ SET PROCESS/NAME=NJOY87
$ SET DEF LOC$DISK ! local scratch disk
$ COPY DKB2:[LEEGE.JEF11]'P2'.DAT 'P2'.DAT ! copy input library to scratch1
$ ASSIGN/USER DKB2:[LEEGE.JEF11]'P2'.DAT TAPE20
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P1'.INP FOR005
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P1'.OUT FOR006
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P2'G0.DAT TAPE26 ! NJOY output
                                         temperature-independent data
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P2'GT.DAT TAPE27 ! NJOY output
                                         temperature-dependent data
$ ASSIGN/USER 'P2'.DAT FOR0901
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P2'X.DAT FOR097 ! NJOY(XLACSR)
                                         output
$ ASSIGN/USER NLA0: FOR047 ! null device
$ SET NOON
$ RUN DKA2:[RFCODE.FINE]NJOY87
$ DELETE FOR0*.DAT;* ! temporary files1
$ DELETE TAPE*.DAT;* ! temporary files
$ DELETE ' P2'.DAT;* ! copy input library1
```

P1 and P2 are parameters which can be used in the VAX/VMS operating system

P1 and P2 are used to create the name of a file

<sup>1</sup>This line can be removed if XLACSR is not used.

## Appendix C

### NJOY input file for sample problem 1: hydrogen in water (different temperatures)

```
0
5
*RECONR*
20 -21
*PENDF TAPE FOR H1 FROM JEF1.1*/
4011 2 /
.001 0. 7/
*H1 FROM JEF1.1*/
*PROCESSED BY THE NJOY NUCLEAR DATA PROCESSING SYSTEM*/
0/
*BROADR*
-21 -22
4011 3 0 0 0.
0.001/
293.6 473.6 623.6 /
0/
*THERMR*
30 -22 -24
4001 4011 8 3 4 0 2 222 0
293.6 473.6 623.6 /
0.01 3.30
*GROUPR*
20 -24 0 -23
4011 10 0 4 3 1 1 1
*H IN H2O*/
293.6 /
1.E10 /
0.10 0.025 0.8203E06 1.40E06/
3/
3 222 *THERMAL*/
3 251 *COS*/
6/
6 222 *THERMAL*/
0/
0/
*GROUPR*
20 -24 0 -25
4011 10 0 4 3 3 1 1
*H IN H2O 3T*/
293.6 473.6 623.6 /
1.E10 /
0.10 0.025 0.8203E06 1.40E06/
3 222 *THERMAL SCAT*/
6 222 *THERMAL SCAT*/
```

0/  
3 222 \*THERMAL SCAT\*/  
6 222 \*THERMAL SCAT\*/  
0/  
3 222 \*THERMAL SCAT\*/  
6 222 \*THERMAL SCAT\*/  
0/  
0/  
\*MODER\*  
-23 26  
\*MODER\*  
-25 27  
\*STOP\*

## Appendix D

NJOY input file for sample problem 2:  $^{235}\text{U}$ , different temperatures and  $\sigma_0$  values

```
0
5
*XACCSR*
AMPX MASTER (SCALE-3)
BASE TEMPERATURE = 293.16, LANL 187 GROUP SET
NUCLIDES FOR LWR
ONLY RESONANCE TREATMENT (MT=1,2,18,102,1023,1022,1021)
IW=2; FISS + 1/E + MAXW.
1$$ 1 1 187 52 2
2$$ 0 80000 210000 250 0 97 0 2 90 0 0 0
3$$ 1 1 0 0 0 0
T
7U
(6E12.5)
2.00000E+07 1.70000E+07 1.60000E+07 1.50000E+07 1.46400E+07 1.44200E+07
1.42000E+07 1.39400E+07 1.37500E+07 1.35000E+07 1.30000E+07 1.20000E+07
1.10000E+07 1.00000E+07 8.82500E+06 7.78800E+06 6.87290E+06 6.06530E+06
5.35260E+06 4.72370E+06 4.16860E+06 3.67880E+06 3.24650E+06 2.86500E+06
2.52840E+06 2.23130E+06 1.96910E+06 1.73770E+06 1.53350E+06 1.35340E+06
1.19430E+06 1.05400E+06 9.30140E+05 8.20850E+05 7.24400E+05 6.39280E+05
5.64160E+05 4.97870E+05 4.39370E+05 3.87740E+05 3.42180E+05 3.01970E+05
2.66490E+05 2.35180E+05 2.07540E+05 1.83160E+05 1.61630E+05 1.42640E+05
1.25880E+05 1.11090E+05 9.80370E+04 8.65170E+04 7.63510E+04 6.73790E+04
5.94620E+04 5.24750E+04 4.63090E+04 4.08680E+04 3.60660E+04 3.18280E+04
2.80880E+04 2.60580E+04 2.47880E+04 2.18750E+04 1.93050E+04 1.70360E+04
1.50340E+04 1.32680E+04 1.17090E+04 1.03330E+04 9.11880E+03 8.04730E+03
7.10170E+03 6.26730E+03 5.53080E+03 4.88100E+03 4.30740E+03 3.80130E+03
3.35460E+03 2.96040E+03 2.61260E+03 2.30560E+03 2.03470E+03 1.79560E+03
1.58460E+03 1.39840E+03 1.23410E+03 1.08910E+03 9.61120E+02 8.48180E+02
7.48520E+02 6.60570E+02 5.82950E+02 5.14450E+02 4.54000E+02 4.00650E+02
3.53580E+02 3.12030E+02 2.75360E+02 2.43010E+02 2.14450E+02 1.89260E+02
1.67020E+02 1.47390E+02 1.30070E+02 1.14790E+02 1.01300E+02 8.93980E+01
7.88930E+01 6.96230E+01 6.14420E+01 5.42220E+01 4.78510E+01 4.22290E+01
3.72670E+01 3.28880E+01 2.90230E+01 2.56130E+01 2.26030E+01 1.99470E+01
1.76030E+01 1.55350E+01 1.37100E+01 1.20990E+01 1.06770E+01 9.42250E+00
8.31530E+00 7.33820E+00 6.86800E+00 6.47600E+00 5.71500E+00 5.04350E+00
4.45090E+00 3.92790E+00 3.46630E+00 3.05900E+00 2.69960E+00 2.38240E+00
2.10240E+00 1.85540E+00 1.72610E+00 1.59490E+00 1.45740E+00 1.30790E+00
1.16640E+00 1.12540E+00 1.09870E+00 1.07220E+00 1.06230E+00 1.05250E+00
1.04270E+00 1.01370E+00 9.92000E-01 9.71000E-01 9.50650E-01 9.10000E-01
8.76420E-01 8.33680E-01 7.82080E-01 6.25060E-01 5.03230E-01 4.14990E-01
3.57670E-01 3.20630E-01 3.01120E-01 2.90740E-01 2.70520E-01 2.51030E-01
2.27690E-01 1.84430E-01 1.52300E-01 1.45720E-01 1.11570E-01 8.19660E-02
6.70000E-02 5.69220E-02 5.00000E-02 4.27550E-02 3.55000E-02 3.06120E-02
2.55000E-02 2.04920E-02 1.23960E-02 6.32470E-03 2.27690E-03 7.60220E-04
```

2.53990E-04 1.00000E-05  
T  
U235 JEF1.1 MATNO=4925 BASE T=293.16K  
70\$ 922350 4925 1 0 0 2 0 1 0  
71\*\* 1.E10 2. 5. 5. 0 0 0 0 0 T  
73\*\* 293.16  
T  
\*RECONR\*  
+20 -22  
\*PENDF TAPE FOR U235 FROM JEF1.1\*/  
4925 2 /  
.001 0. 7/  
\*U235 FROM JEF1.1\*/  
\*PROCESSED BY THE NJOY NUCLEAR DATA PROCESSING SYSTEM\*/  
0/  
\*BROADR\*  
-22 -23  
4925 3 0 0 0.  
0.001/  
293.16 900. 1500.  
0/  
\*UNRESR\*  
+20 -23 -22  
4925 3 3 0  
293.16 900. 1500.  
1.E10 500. 1.  
0/  
\*THERMR\*  
0 -22 -24  
0 4925 8 3 1 0 1 221 0  
293.16 900. 1500.  
0.01 3.30  
\*GROUPR\*  
20 -24 0 -23  
4925 10 0 4 3 1 1 1  
\*U235 JEF 1.1 1T 1S0\*/  
293.16  
1.E10  
0.10 0.025 0.8203E06 1.4E06 /  
3/  
3 221 \*FREE THERMAL\*/  
3 251 \*MUBAR\*/  
3 252 \*XI\*/  
3 253 \*G\*/  
3 452 \*NU\*/  
6/  
6 221 \*FREE THERMAL\*/  
0/  
0/  
\*GROUPR\*  
20 -24 0 -25  
4925 10 0 4 3 3 3 1  
\*U235 JEF 1.1 3T 3S0\*/

293.16 900. 1500.  
1.E10 500. 1.  
0.10 0.025 0.8203E06 1.4E06 /  
3 1 \*TOTAL\*/  
3 2 \*SCAT\*/  
3 18 \*FIS\*/  
3 102 \*CAPT\*/  
3 221 \*THERMAL\*/  
6 221 \*THERMAL SCATTERING\*/  
0/  
3 1 \*TOTAL\*/  
3 2 \*SCAT\*/  
3 18 \*FIS\*/  
3 102 \*CAPT\*/  
3 221 \*THERMAL\*/  
6 221 \*THERMAL SCATTERING\*/  
0/  
3 1 \*TOTAL\*/  
3 2 \*SCAT\*/  
3 18 \*FIS\*/  
3 102 \*CAPT\*/  
3 221 \*THERMAL\*/  
6 221 \*THERMAL SCATTERING\*/  
0/  
0/  
\*MODER\*  
-23 26  
\*MODER\*  
-25 27  
\*STOP\*

## Appendix E

### Command file (VAX/VMS) to run MILER

```
$ SET PROCESS/NAME=MILER.T
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P1'M.OUT FOR006
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]MILER.INP FOR005
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P1'M.DAT FOR030 ! MILER output
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P1'G0.DAT FOR022 ! NJOY output
                           temperature-independent data
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P1'GT.DAT FOR023 ! NJOY output
                           temperature-dependent data
$ SET NOON
$ SET DEF LOC$DISK ! local scratch disk
$ RUN DKA2:[RFCODE.FINE]MILER
$ DELETE FOR0*.DAT;* ! temporary files
```

## Appendix F

### MILER input file for sample problems 1 and 2

22 23 -30 0 90  
0/

P1 is a parameter which can be used in the VAX/VMS operating system

P1 is used to create the name of a file

## **Appendix G**

### **Command file (VAX/VMS) to run UNITABR**

```
$ SET PROCESS/NAME=UNITABR  
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P1'MM.DAT FOR001 ! output UNITABR  
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P1'U.INP FOR005  
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P1'U.OUT FOR006  
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P1'X.DAT FOR023 ! XLACSR output  
$ ASSIGN/USER DKB2:[LEEGE.NSLINK]'P1'M.DAT FOR024 ! MILER output  
$ SET DEF LOC$DISK ! local scratch disk  
$ SET NOON  
$ RUN DKA2:[RFCODE.UTIL]UNITABR  
$ DELETE FOR0*.DAT;* ! temporary files
```

## **Appendix H**

### **UNITABR input file for sample problem 2**

```
1$$ 1 2  
6$$ 200 880  
T  
2$$ 92235 23 922350 5555  
    92235 24    4925 1111  
T
```

P1 is a parameter which can be used in the VAX/VMS operating system

P1 is used to create the name of a file

# **Appendix I**

## **Contents of tape**

**Characteristics:** density = 6250 bpi, ascii, nolabel, recordformat=fixed, blocked, recordsize = 80, blocksize =3200, (output: recordsize = 133, blocksize = 5320)

1. NJOY87 main source (FORTRAN)
2. XLACSR source (FORTRAN)
3. MILER (extensively revised) source (FORTRAN)
4. UNITABR source (FORTRAN)
5. BONAMI subroutines (BFEDIT, CAPY, MAST and SELECT) source (FORTRAN)
6. Sample problem 1 input file NJOY87
7. Sample problem 2 input file NJOY87 including XLACSR
8. Sample problem 1 and 2 input file MILER
9. Sample problem 2 input file UNITABR
10. Sample problem 1 output file NJOY87
11. Sample problem 2 output file NJOY87 including XLACSR
12. Sample problem 1 output file MILER
13. Sample problem 2 output file MILER
14. Sample problem 2 output file UNITABR
15. Sample problem 1 and 2 command file NJOY87 (including XLACSR)
16. Sample problem 1 and 2 command file MILER
17. Sample problem 2 command file UNITABR